Electron Phonon Interaction In Low Dimensional Structures Series On Semiconductor Science And Technology

This second, thoroughly revised, updated and enlarged edition provides a straightforward introduction to spectroscopy, showing what it can do and how it does it, together with a clear, integrated and objective account of the wealth of information that may be derived from spectra. It also features new chapters on spectroscopy in nano-dimensions, nano-optics, and polymer analysis. Clearly structured into sixteen sections, it covers everything from spectroscopy in nanodimensions to medicinal applications, spanning a wide range of the electromagnetic spectrum and the physical processes involved, from nuclear phenomena to molecular rotation processes. In addition, data tables provide a comparison of different methods in a standardized form, allowing readers to save valuable time in the decision process by avoiding wrong turns, and also help in selecting the instrumentation and performing the experiments. These four volumes are a must-have companion for daily use in every lab.

These notes are a result of a series of lectures given to the MS and PhD students of the Department of Physics, Moscow State Pedagogical University. They deal with the subject of electron-phonon interaction in pure threedimensional metals. The goal was to show how one could calculate the temperature dependence of the electron-phonon-interaction time from first principles within a simple model. Students wishing to expand their knowledge of the subject of condensed matter are invited to study any book on solid-state physics (for example by J.M. Ziman, or N.W. Ashcroft and N.D. Mermin.

Understanding the mechanism of the high-temperature superconductors has been a very important topic in condensed matter physics. Researchers have been trying to explain the role of electron-phonon interaction (EPI) in cuprates. Some important properties of the cuprates could not be explained by conventional BCS theory. This book contains the experimental and theoretical studies on the EPI. The experimental part covers the results of angle-resolved photoemission spectroscopy (ARPES), isotopic effect, elastic neutron scattering study of electron-phonon, lattice role and so on. The theoretical part covers the electron-phonon, polaron and bipolaron, effect of lattice, fine structure in the tunnelling spectra of electron-doped cuprates, identification of the bulk pairing symmetry in high-temperature superconductors.Students and researchers interested in high-temperature superconductors, especially the EPI in cuprates will find this title very useful.

Quantum mechanical laws are well documented at the level of a single or a few atoms and are here extended to systems containing 102 to 1010 electrons - still much smaller than the usual macroscopic objects, but behaving in a manner similar to a single atom. Besides the purely theoretical interest, such systems pose a challenge to the achievement of the ultimate microelectronic applications. The present volume presents an up-to-date account of the physics, technology and expected applications of quantum effects in solid-state mesoscopic structures. Physical phenomena include the Aharonov-Bohm effect, persistent currents, Coulomb blockade and Coulomb oscillations in single electron devices, Andreev reflections and the Josephson effect in superconductor/normal/superconductor systems, shot noise suppression in microcontacts and contact resistance quantisation, and overall quantum coherence in mesoscopic and nanoscopic structures related to the emerging physics of quantum computation in the solid-state environment.

This monograph is a radical departure from the conventional quantum mechanical approach to electron-phonon interactions. It translates the customary quantum mechanical analysis of the electron-phonon interactions carried out in Fourier space into a predominantly classical analysis carried out in real space. Various electron-phonon interactions such as the polar and nonpolar optical phonons, acoustic phonons that interact via deformation potential and via the piezoelectric effect and phonons in metals, are treated in this monograph by a single, relatively simple ?classical? model. This model is shown to apply to electron interactions with the deep lying X-ray levels of atoms, with plasmons and with Cerenkov radiation. The unifying concept that applies to all of these phenomena is a new definition of a coupling constant. The essentially classical interaction of an electron with its surrounding is clearly brought out to be the cause of spontaneous emission of phonons. The same concept also applies to the case of spontaneous emission of photons. While the bulk of this monograph deals with quanta of phonons and quanta of photons, a discussion of the acousto electric effect which is a purely classical phenomenon is presented. The newly defined coupling constant turns out to be valid too for this discussion. This universality of the coupling constant goes far beyond. It is equally applicable to amorphous materials. This significant application gives an analytic formulation of mobility in amorphous materials.

This is a classic text of its time in condensed matter physics.

Design, Fabrication, and Characterization of Multifunctional Nanomaterials covers major techniques for the design, synthesis, and development of multifunctional nanomaterials. The chapters highlight the main characterization techniques, including X-ray diffraction, scanning electron microscopy, high-resolution transmission electron microscopy, energy dispersive X-ray spectroscopy, and scanning probe microscopy. The book explores major synthesis methods and functional studies, including: Brillouin spectroscopy; Temperature-dependent Raman spectroscopic studies; Magnetic, ferroelectric, and magneto-electric coupling analysis; Organ-on-a-chip methods for testing nanomaterials; Magnetron sputtering techniques; Pulsed laser deposition techniques; Positron annihilation spectroscopy to prove defects in nanomaterials; Electroanalytic techniques. This is an important reference source for materials science students, scientists, and engineers who are looking to increase their understanding of design and fabrication techniques for a range of multifunctional nanomaterials. Explains the major design and fabrication techniques and processes for a range of multifunctional nanomaterials; Demonstrates the design and development of magnetic, ferroelectric, multiferroic, and carbon nanomaterials for electronic applications, energy generation, and storage; Green synthesis techniques and the development of nanofibers and thin films are also emphasized.

These proceedings cover the possible manifestations of electron-phonon interactions in understanding high Tc superconductivity. The results of measurements of different experimental methods have been analysed, and the role played by electrons in superconductivity, taking into account the van Hove singularity, has also been discussed. The pairing of electrons by other bosonic excitations, as well as the effects of strong local electron-lattice interactions are reviewed. Another important point is the ab initio calculations discussed by several authors that remark the importance of electron-phonon effects for high Tc superconductivity.

Nanotechnology is a 'catch-all' description of activities at the level of atoms and molecules that have applications in the real world. A nanometer is a billionth of a meter, about 1/80,000 of the diameter of a human hair, or 10 times the diameter of a hydrogen atom. Nanotechnology is now used in precision engineering, new materials development as well as in electronics; electromechanical systems as well as mainstream biomedical applications in areas such as gene therapy, drug delivery and novel drug discovery techniques. This new book presents the latest research from around the world on nanorods, nanotubes and nanomaterials.

This two-volume work covers ultrafast structural and electronic dynamics of elementary processes at solid surfaces and interfaces, presenting the current status of photoinduced processes. Providing valuable introductory information for newcomers to this booming field of research, it investigates concepts and experiments, femtosecond and attosecond time-resolved methods, as well as frequency domain techniques. The whole is rounded off by a look at future developments.

Magnetic and superconducting materials pervade every avenue of the technological world – from microelectronics and mass-data storage to medicine and heavy engineering. Both areas have experienced a recent revitalisation of interest due to the discovery of new materials, and the re-evaluation of a wide range of basic mechanisms and phenomena. This Concise Encyclopedia draws its material from the award-winning Encyclopedia of Materials and Engineering, and includes updates and revisions not available in the original set -- making it the ideal reference companion for materials scientists and engineers with an interest in magnetic and superconducting materials. * Contains in excess of 130 articles, taken from the award-winning Encyclopedia of Materials: Science and Technology, including ScienceDirect updates not available in the original set. * Each article discusses one aspect of magnetic and superconducting materials and includes photographs, line drawings and tables to aid the understanding of the topic at hand. * Cross-referencing guides readers to articles covering subjects of related interest.

The book describes how the electrons in small "low-dimensional" structures interact with their surroundings. It contains a series of linked up to date review chapters as well as explanatory material and is written to be understandable to graduate students and newcomers to the field. All contributions come from leading scientists.

This is a combined volume of the Proceedings for the Workshop on 'Mechanisms of High Tc Superconductivity' (20 June –29 July) and the Adriatico Research Conference (26 - 29 July) on high temperature superconductivity. It aims to bring together a critical overview of the experimental situation and an in-depth discussion of the various theoretical models proposed to explain the mechanisms for high temperature superconductivity by experts actively involved in high Tc research.

Papers presented at the International Conference on Phonons in Condensed Materials, held at Bhopal during 20-23 January 2003.

The structural. electronic and lattice properties of superconducting ternary com pounds are the subject of this Topics volume. Its companion volume (Topics in Cur rent Physics. Volume 34) deals primarily with the mutual interaction of supercon ductivity and magnetism in ternary compounds. These two volumes are the culmination of a project. started nearly two years ago. that was inspired by the intense re search effort. both experimental and theoretical. then being expended to explore and develop an understanding of the remarkable physical properties of ternary super conductors. Research activity on this subject has increased in the meantime. The interest in ternary superconductors originated in 1972. when B.T. Matthias and his co-workers first discovered superconductivity in several ternary molybdenum sulfide compounds that had been synthesized in 1971 by R. Chevrel. M. Sergent. and J. Prigent. The superconducting critical temperature Tc of one of the compounds. PbMo S • was reported to be ~ 15 K. This value is sufficiently high that there was g 6 (and still is) reason to expect that other ternary compounds would be found with superconducting transition temperatures rivaling those of the A15 compounds. of which Nb Ge has the record high Tc of 23 K. The interest in ternary superconductors 3 received further impetus when several of the ternary molybdenum sulfides were found to have exceptionally high upper critical magnetic fields. some of them in the neighborhood of 50 Tesla or more. An immense amount of research on ternary molybdenum chalcogenides then followed.

The generation and propagation of pulses of nonequilibrium acoustic phonons and their interaction with semiconductor nanostructures are investigated. Such studies can give unique information about the properties of low-dimensional electron systems, but in order to interpret the experiments and to understand the underlying physics, a comparison with theoretical models is absolutely necessary. A central point of this work is therefore a universal theoretical approach allowing the simulation and the analysis of phonon spectroscopy measurements on low-dimensional semiconductor structures. The model takes into account the characteristic properties of the considered systems. These properties are the elastic anisotropy of the substrate material leading to focusing effects and highly anisotropic phonon propagation, the anisotropic nature of the different electron-phonon coupling mechanisms, which depend manifestly on phonon wavevector direction and polarization vector, and the sensitivity to the confinement parameters of the low-dimensional electron systems. We show that screening of the electron-phonon interaction can have a much stronger influence on the results of angle-resolved phonon spectroscopy than expected from transport measurements. Since we compare theoretical simulations with real experiments, the geometrical arrangement and the spatial extension of phonon source and detector are also included in the approach enabling a quantitative analysis of the data this way. To illustrate the influence of acoustic anisotropy and carrier confinement on the results of phonon spectroscopy in detail we analyse two different applications. In the first case the low-dimensional electron system acts as the phonon detector and the phonon induced drag current is measured. Our theoretical model enables us to calculate the electric current induced in low-dimensional electron systems by pulses of (ballistic) nonequilibrium phonons. The theoretical drag patterns reproduce the main featu.

The NATO Advanced Research Workshop took place from 29 May to I June 2000 in the picturesque Hungarian town of Pecs, 220 km south of Budapest. The main goal of the workshop was to review and promote experimental and theoretical research on the problem of Kondo-type scatteringofthe electrons in systems ofreduced dimensionalities. 53 regular participants and 7 observers from 17 different countries attended the workshop. The Kondo effect has been a topic ofintense interest for many years, due in part to its relevance to a variety of other branches of condensed matter physics. In addition to the best known example of magnetic impurities in noble metals, the physics of the Kondo effect is important in many areas of current research, including heavy-fermion physics, correlated electron systems, and high-temperature superconductivity. Of central importance in this problem is the interaction of conduction electrons in the metal with individual magnetic impurities, an interaction which also mediates the interaction ofthe impurities with each other.

PhD students, academics, researchers and industrialists in nanotechnology.

The characteristics of electrical contacts have long attracted the attention of researchers since these contacts are used in every electrical and electronic device. Earlier studies generally considered electrical contacts of large dimensions, having regions of current concentration with diameters substantially larger than the characteristic dimensions of the material: the interatomic distance, the mean free path for electrons, the coherence length in the superconducting state, etc. [110]. The development of microelectronics presented to scientists and engineers the task of studying the characteristics of electrical contacts with ultra-small dimensions. Characteristics of point contacts such as mechanical stability under continuous current loads, the magnitudes of electrical fluctuations, inherent sensitivity in radio devices and nonlinear characteristics in connection with electromagnetic radiation can not be understood and altered in the required way without knowledge of the physical processes occurring in contacts. Until recently it was thought that the electrical conductivity of contacts with direct conductance (without tunneling or semiconducting barriers) obeyed Ohm's law. Nonlinearities of the current-voltage characteristics were explained by joule heating of the metal in the region of the contact. However, studies of the current-voltage characteristics of metallic point contacts at low (liquid helium) temperatures [142] showed that heating effects were negligible in many cases and the nonlinear characteristics under these conditions were observed to take the form of the energy dependent probability of inelastic electron scattering, induced by various mechanisms.

Lasers are playing a more and more dominant role in modern optical spec troscopy, offering an increased potential for high resolution and, thus, for more detailed spectroscopic information on dynamic and structural param eters. This book on Zero-Phonon Lines and Spectral Hole Burning in Spec troscopy and Photochemistry gives a concise and very useful survey of some of the pioneering and current work on solid state spectroscopy of various groups in the USSR. It focusses on the optical Mossbauer analogue, the "zero-phonon line", and "hole burning" spectroscopy, a method which increases the resolu tion well beyond the zero-phonon linewidth. In this conte. . 'Ct, the present work is complementary to Persistent Spectral Hole-Burning: Science and Applica tions (ed. by W.E. Moerner, Springer, Berlin, Heidelberg 1988), which deals in more detail with the various aspects of laser spectroscopy with ultrahigh spectral resolution. Zero-phonon lines and an understanding of the various phonon coupling mechanisms which are treated in this book are a prerequi site for applying and understanding techniques of ultrahigh resolution such as hole-burning or optical echoes. Bayreuth, March 1988 D. Haarer Preface The investigation of zero-phonon lines (ZPLs) is one of the foremost and most informative fields of present-day condensed-matter spectroscopy. Along with its definite function in physical cognition and investigation methods, the spectroscopy of ZPLs is also gaining purely practical applications. This is due to the fact that ZPLs are extra-sensitive quantum-mechanical detectors.

This Briefs volume describes the properties and structure of elementary excitations in isotope low-dimensional structures. Without assuming prior knowledge of quantum physics, the present book provides the basic knowledge needed to understand the recent developments in the sub-disciplines of nanoscience isotopetronics, novel device concepts and materials for nanotechnology. It is the first and comprehensive interdisciplinary account of the newly developed scientific discipline isotopetronics.

The article is a study of the change in the characteristics of the phonon spectrum as a function of the magnetic field. This change is particularly marked with strong magnetic fields, since the change in the Fermi surface in this case is considerable. The calculation is carried out by the known method of Green's functions at a temperature of absolute zero. Practically speaking, it is a question of temperatures much lower than the electron degeneracy temperature and the Debye temperature. To find the phonon spectrum, a solution is found to the Dyson equation for the Green's function of the phonon. On the above basis, the author proceeds to a mathematical solution of the problem posed.

Presently, there is an intense race throughout the world to develop good enough thermoelectric materials which can be used in wide scale applications. This book focuses comprehensively on very recent up-to-date breakthroughs in thermoelectrics utilizing nanomaterials and methods based in nanoscience. Importantly, it provides the readers with methodology and concepts utilizing atomic scale and nanoscale materials design (such as superlattice structuring, atomic network structuring and properties control, electron correlation design, low dimensionality, nanostructuring, etc.). Furthermore, also indicates the applications of thermoelectrics expected for the large emerging energy market. This book has a wide appeal and application value for anyone being interested in state-of-the-art thermoelectrics and/or actual viable applications in nanotechnology.

Superconductivity in Highly Correlated Fermion Systems documents the proceedings of the Yamada Conference XVIII on Superconductivity in Highly Correlated Fermion Systems held in Sendai, Japan, from August 31 to September 3, 1987. This book compiles selected papers on the experimental and theoretical advances in the study of superconductivity. The topics include the superconductivity and magnetism in heavy-electron materials, magneto-resistance of heavy-fermion compounds, and magnetic fluctuations and order in exotic superconductors. The fabrication and properties of thin superconducting oxide films, bipolaron models of superconductors, superconducting properties of superlattices, and flux quantization on quasi-crystalline networks are also covered. This publication is recommended for physicists and students researching on the superconductivity in highly correlated fermion systems.

This third edition of the Encyclopedia of Spectroscopy and Spectrometry provides authoritative and comprehensive coverage of all aspects of spectroscopy and closely related subjects that use the same fundamental principles, including mass spectrometry, imaging techniques and applications. It includes the history, theoretical background, details of instrumentation and technology, and current applications of the key areas of spectroscopy. The new edition will include over 80 new articles across the field. These will complement those from the previous edition, which have been brought up-to-date to reflect the latest trends in the field. Coverage in the third edition includes: Atomic spectroscopy Electronic spectroscopy Fundamentals in spectroscopy High-Energy spectroscopy Magnetic resonance Mass spectrometry Spatially-resolved spectroscopic analysis Vibrational, rotational and Raman spectroscopies The new edition is aimed at professional scientists seeking to familiarize themselves with particular topics quickly and easily. This major reference work continues to be clear and accessible and focus on the fundamental principles, techniques and applications of spectroscopy and spectrometry. Incorporates more than 150 color figures, 5,000 references, and 300 articles for a thorough examination of the field Highlights new research and promotes innovation in applied areas ranging from food science and forensics to biomedicine and health Presents a one-stop resource for quick access to answers and an in-depth examination of topics in the spectroscopy and spectrometry arenas

In the last ten years, the physics and technology of low dimensional structures has experienced a tremendous development. Quantum structures with vertical and lateral confinements are now routinely fabricated with feature sizes below 100 run. While quantization of the electron states in mesoscopic systems has been the subject of intense investigation, the effect of confinement on lattice vibrations and its influence on the electron-phonon interaction and energy dissipation in nanostructures received atten tion only recently. This NATO Advanced Research Workshop on Phonons in Sem iconductor Nanostructures was a forum for discussion on the latest developments in the physics of phonons and their impact on the electronic properties of low-dimensional structures. Our goal was to bring together specialists in lattice dynamics and nanos tructure physics to assess the increasing importance of phonon effects on the physical properties of one-(lD) and zero-dimensional (OD) structures. The Workshop addressed various issues related to phonon physics in III-V, II-VI and IV semiconductor nanostructures. The following topics were successively covered: Models for confined phonons in semiconductor nanostructures, latest experimental observations of confined phonons and electron-phonon interaction in two-dimensional systems, elementary excitations in nanostructures, phonons and optical processes in reduced dimensionality systems, phonon limited transport phenomena, hot electron effects in quasi - ID structures, carrier relaxation and phonon bottleneck in quantum dots.

Remarkable developments in the spectroscopy field regarding ultrashort pulse generation have led to the possibility of producing light pulses ranging from 50 to5 fs and frequency tunable from the near infrared to the ultraviolet range. Such pulses enable us to follow the coupling of vibrational motion to the electronic transitions in molecules and solids in real time. Detailing these advanced developments, as well as the fundamental methods and tools of vibrational spectroscopy, Coherent Vibrational Dynamics providesresearchers and students with a uniquely comprehensive resource. With the contributions of pioneering scientists, this seminal volume – · Outlines the principles and tools used on time-domain vibrational spectroscopy and provides a general introduction to the subject of coherent phonons · Describes the modern methods for tunable ultrashort pulse generation from infrared to visible-UV · Reviews coherent vibrational dynamics in small molecules in liquids (hydrogen bonds), and in carbon based conjugated materials (polyenes, carotenoids, and semiconducting polymers) · Explores phonon dynamics in semiconductors (bulk and heterostructures) and in quasi-one-dimensional systems Supplemented with a great number of references, and covering fundamental as well advanced topics, this text provides a valuable reference for both graduate students and senior researchers investigating materials in physics, chemistry, and biology. It is also an excellent starting point for those who want to pursue research in the field of ultrafast optics and spectroscopy.

This NATO Advanced Study Institute was the fourth in a series devoted to the subject of phase transitions and instabilities with particular attention to structural phase transforma~ions. Beginning wi th the first Geilo institute in 19'(1 we have seen the emphasis evolve from the simple quasiharmonic soft mode description within the Landau theory, through the unexpected spectral structure re presented by the "central peak" (1973), to such subjects as melting, turbulence and hydrodynamic instabilities (1975). Sophisticated theoretical techniques such as scaling laws and renormalization group theory developed over the same period have brought to this wide range of subjects a pleasing unity. These institutes have been instrumental in placing structural transformations clearly in the mainstream of statistical physics and critical phenomena. The present Geilo institute retains some of the counter cul tural flavour of the first one by insisting whenever possible upon peeking under the skirts of even the most successful phenomenology to catch a glimpse of the underlying microscopic processes. Of course the soft mode remains a useful concept, but the major em phasis of this institute is the microscopic cause of the mode softening. The discussions given here illustrate that for certain important classes of solids the cause lies in the electron phonon interaction. Three major types of structural transitions are considered. In the case of metals and semimetals, the electron phonon interaction relie6 heavily on the topology of the Fermi surface.

The study of electrons and holes confined to two, one and even zero dimensions has uncovered a rich variety of new physics and applications. This book describes the interaction between these confined carriers and the optic and acoustic phonons within and around the confined regions.

This book contains lectures delivered at the 10th Physics Summer School on “Physics of Novel Materials” at Australian National University by internationally reputed scientists. It covers a wide variety of materials: semiconductors, superconductors, polymers, zeolites, clusters and nanostructures, and transport in novel materials. It is hard to find theoretical and experimental aspects of such diverse topics on novel materials in a single volume. Contents:The Electronic and Structural Properties of Semiconductor Clusters and Nanostructures (J R Chelikowsky)Classical and High Temperature Superconductivity (J H Miller Jr. & J R Claycomb)Electrons Solvated in Zeolites (N P Blake & H Metiu)Spin Glasses (D Sherrington)The Wonderful World of Carbon (S Prawer)Semiconductor Heterostructures (R G Elliman)Ion Implantation: A Nonequilibrium Process (J S Williams)Transport in Novel Materials (A B Kaiser)Coherent Wave Transport in Low Dimensional Random Media (N Kumar) Readership: Condensed matter physicists and materials scientists. Keywords:

The problem of conventional, low-temperature superconductivity has been regarded as solved since the seminal work of Bardeen, Cooper, and Schrieffer (BCS) more than 50 years ago. However, the theory does not allow accurate predictions of some of the most fundamental properties of a superconductor, including the superconducting energy gap on the Fermi surface. This thesis describes the development and scientific implementation of a new experimental method that puts this old problem into an entirely new light. The nominee has made major contributions to the development and implementation of a new experimental method that enhances the resolution of spectroscopic experiments on dispersive lattice-vibrational excitations (the "glue" responsible for Cooper pairing of electrons in conventional superconductors) by more than two orders of magnitude. Using this method,he has discovered an unexpected relationship between the superconducting energy gap and the geometry of the Fermi surface in the normal state, both of which leave subtle imprints in the lattice vibrations that could not be resolved by conventional spectroscopic methods. He has confirmed this relationship on two elemental superconductors and on a series of metallic alloys. This indicates that a mechanism qualitatively beyond the standard BCS theory determines the magnitude and anisotropy of the superconducting gap.

Contents:Lattice Vibrations of the Cuprate Superconductors (W Reichardt et al)Evidence of Strong Electron-Phonon Interaction from the Infrared Spectra of YBa2Cu3O7 (T Timusk & D B Tanner)Electron-Phonon Interaction and Infrared Spectra of High Temperature Superconductors (O V Dolgov et al)Tunneling Studies of Bimuthate and Cuprate Superconductors (J F Zasadzinski et al)Phonon Mechanism of the High Tc Superconductivity Based on the Tunneling Structure (D Shimada et al)Lattice Instabilities in High Temperature Superconductors: The X Tilt Point Energy Surface for La2-xBaxCuO4 (W E Pickett et al)Structural Instability and Strong Coupling in Oxide Superconductors (N M Plakida)On the Isotope Effect (J P Carbotte)Electron-Phonon Coupling, Oxygen Isotope Effect and Superconductivity in Ba1-xKxBio3 (C K Loong et al)Weak Coupling Theory of the High-Tc Superconductors Based on the Electron-Phonon Interaction (J Labbé)Phonon Self-Energy Effects in Migdal-Eliashberg Theory (F Marsiglio)Electron-Phonon Interaction and Superconductivity in BaxK1-xBiO3 (K Motizuki et al)The Effect of Strong Coulomb Correlations on Electron-Phonon Interactions in the Copper Oxides: Implications for Transport (J H Kim et al)Zinc Substitution Effects on the Superconducting Properties for Ld1.85Ce0.15CuO4-? (V García-Vázquez et al)Manifestations of the e-ph Interaction: A Summary (R Baquero) Readership: Condensed matter physicists, applied physicists, chemists, electrical engineers and materials scientists. keywords:

Electron-phonon Interactions in Low-dimensional StructuresOxford University Press on Demand

Thermoelectric materials, which enable direct conversion between thermal and electrical energy, provide an alternative for power generation and refrigeration. The key parameter that defines the efficiency of thermoelectric materials is the 'dimensionless figure of merit' ZT, which is composed of the Seebeck coefficient, electrical conductivity and total thermal conductivity respectively. Ideally, to achieve high ZT both the Seebeck coefficient and electrical conductivity should be large, while total thermal conductivity must be minimized. In this thesis, first-principles calculations of the Seebeck coefficient, lattice thermal conductivity and electrical conductivity are performed to study mechanisms and factors that gives rise to high ZT. One effective way to enhance ZT is through direct reduction of lattice thermal conductivity. We perform calculation and analysis of lattice thermal conductivity for thermoelectric materials by solving the Boltzmann transport equation iteratively in the framework of perturbation theory. The second- and third-order interatomic force constants are extracted using the recently developed CSLD (compressive sensing lattice dynamics) method. Afterwards, we evaluate opportunities to achieve further reduction of lattice thermal conductivity. Our first study of ternary zinc-blende-based mineral compounds famatinite (Cu3SbS4) and permingeatite (Cu3SbSe4) shows that optical modes in these two compounds contribute a sizable portion of the total lattice thermal conductivity and thus cannot be neglected. Due to the fact that phonon modes with mean free paths larger than 10 nm carry about 80% of the heat, nanostructuring, which reduces the mean free path, is a promising way to reduce the lattice thermal conductivity by reducing the characteristic length. In addition, our simple alloying model including mass disorder reproduces experimental findings that forming solid solutions rapidly decreases the lattice thermal conductivity. An alternative way to reduce lattice thermal conductivity is to introduce guest atoms in host cage structures. Our study of type-I Si clathrates containing guest atoms Na and Ba shows that Na tends to form incoherent localized phonon mode while Ba coherently couples with the host cages. The low lattice thermal conductivities of Na- and Ba-filled Si clathrates should be attributed to the dramatic reductions in both phonon lifetime and group velocity. Analysis of phonon scattering process reveals that localized modes can be effectively emitted and absorbed, thus dramatically enhancing overall scattering rates. Another widely adopted approach to achieve high ZT is through maintaining a high power factor. To accurately determine the Seebeck coefficient and electrical conductivity, we estimate carrier lifetime due to electron-phonon interaction under relaxation time approximation using the electron-phonon Wannier interpolation technique. Our study of noble metals Cu and Ag shows that their positive Seebeck coefficients can be mostly attributed to the negative energy dependence of carrier lifetime. In contrast to the previous study of positive Seebeck in Li, which is due to the deviation of electronic behavior from that in free electron model, it is the nontrivial energy dependence of electron-phonon interaction vertex that leads to the positive Seebeck coefficient. Intermetallic compound B20-type CoSi has drawn considerable attention due to its exceptionally high power factor and large Seebeck coefficient. Our study shows that the large negative Seebeck coefficient of the pristine CoSi is mostly due to the strong energy dependence of carrier lifetime, which together with the high electrical conductivity leads to the high power factor. For heat transport, both electron-phonon and phonon-phonon interactions contribute significantly to phonon scattering at temperatures lower than 200 K. While at temperatures higher than 300 K, phonon-phonon interaction dominates over electron-phonon interaction. Based on the optimized power factor with properly adjusted carrier concentration, we predict that the maximum ZTs at 300 and 600 K are about 0.11 and 0.25 respectively without further reducing the total thermal conductivity. Known good thermoelectric materials often are comprised of elements that are in low abundance, toxic and require careful doping and complex synthesis procedures. High performance thermoelectricity has been reported in earth-abundant compounds based on natural mineral tetrahedrite (Cu12Sb4S13). Our first-principles electronic structure calculations of Cu12Sb4S13 show that Cu atoms are all in the monovalent state, creating two free hole states per formula unit of the pristine compound. Optimal thermoelectric performance can be achieved via electron doping. Substituting transition metals on Cu 12d sites does the job. Detailed analysis shows that Zn and Fe substitutions tend to fill the empty hole states, while Ni substitution introduces an additional hole to the valence band by forming ferromagnetic configuration. Experimentally observed extremely low lattice thermal conductivity can be attributed to the out-of-plane vibrations of the three-fold Cu ions. This is further verified by the large Gruneisen parameter calculated.

The field of low-dimensional structures has been experiencing rapid development in both theoretical and experimental research. Phonons in Low Dimensional Structures is a collection of chapters related to the properties of solid-state structures dependent on lattice vibrations. The book is divided into two parts. In the first part, research topics such as interface phonons and polaron states, carrier-phonon non-equilibrium dynamics, directional projection of elastic waves in parallel array of N elastically coupled waveguides, collective dynamics for longitudinal and transverse phonon modes, and elastic properties for bulk metallic glasses are related to semiconductor devices and metallic glasses devices. The second part of the book contains, among others, topics related to superconductor, phononic crystal carbon nanotube devices such as phonon dispersion calculations using density functional theory for a range of superconducting materials, phononic crystal-based MEMS resonators, absorption of acoustic phonons in the hyper-sound regime in fluorine-modified carbon nanotubes and single-walled nanotubes, phonon transport in carbon nanotubes, quantization of phonon thermal conductance, and phonon Anderson localization.

A distinctive introduction to the principles governing polaron science for experimental and theoretical graduate students and researchers.